# Fluid Wet Solid Interfaces Under Pressure --
# Molecular Simulations of Dynamic Fluid Structure

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Solids with solubility in water that increases with pressure will preferentially dissolve at points of contact with other solids when the solid contacts are at higher pressure than the fluid pressure. If the water -- solid system is closed and saturated, material will dissolve at the contacts and be transported out of the contact and precipitated elsewhere. This process, in geosciences known as pressure solution, is the main process responsible for converting sediments into sedimentary rocks and it is thought to be important in healing the strength of faults in earthquake zones. Sedimentary rocks are a class of what have been described as ``mesoscopically elastic'' materials. The elasticity of such materials does not only depend on the bulk elasticity of its constituents, but also on the bond structure. The bond structure -- the properties of the contacts and the distribution of contacts in an aggregate -- is forged by pressure solution and is thought to cause the observed (nonlinear) hysteretic elasticity of such rocks.

Computer simulation has already proven to be a good tool for the study of confined fluids. Many studies of confined films under pressure suggest that they are in a solid-like structure. Since most studies have been directed at understanding the solvatation force and rheological behaviour of fluid films in idealized geometries, studies of diffusion mechanisms in such films are lacking but necessary to understand the fundamentals of pressure solution.

We develop a methodology for grand canonical Monte Carlo preparation of the initial configurations for molecular dynamics simulations of confined fluids at geological conditions. We define projections of the density-density time correlation function in a confined geometry and their connections to the static fluid structure and diffusion. We measure these quantities at different thermodynamic conditions corresponding to different burial depths. A solid surface undergoing pressure solution must have a minimal roughness of atomic dimensions. We study the effect of atomic scale surface irregularities on breaking the crystalline-like film structure locally.